Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2025 – 12:17 PM EDT

PDB ID	:	9DGO / pdb_00009dgo
Title	:	Designed miniproteins potently inhibit and protect against MERS-CoV. Crystal structure of MERS-CoV S RBD in complex with miniprotein cb3
Authors	:	Tortorici, M.A.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2024-09-03
Resolution	:	1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

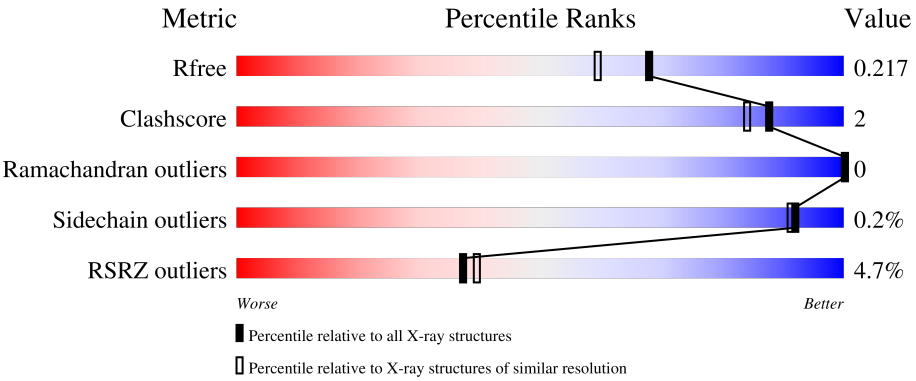
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	258	4% 76% 5% 19%
1	B	258	3% 78% 5% 18%
2	C	58	5% 95% 5%
2	D	58	5% 95%

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Mol	Chain	Length	Quality of chain
3	E	2	100%
4	F	3	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4492 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	2	0
			1568	996	253	308	11			
1	B	212	Total	C	N	O	S	0	4	0
			1630	1032	263	324	11			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	MET	-	initiating methionine	UNP A0A0U2GPS7
A	351	GLY	-	expression tag	UNP A0A0U2GPS7
A	352	ILE	-	expression tag	UNP A0A0U2GPS7
A	353	LEU	-	expression tag	UNP A0A0U2GPS7
A	354	PRO	-	expression tag	UNP A0A0U2GPS7
A	355	SER	-	expression tag	UNP A0A0U2GPS7
A	356	PRO	-	expression tag	UNP A0A0U2GPS7
A	357	GLY	-	expression tag	UNP A0A0U2GPS7
A	358	MET	-	expression tag	UNP A0A0U2GPS7
A	359	PRO	-	expression tag	UNP A0A0U2GPS7
A	360	ALA	-	expression tag	UNP A0A0U2GPS7
A	361	LEU	-	expression tag	UNP A0A0U2GPS7
A	362	LEU	-	expression tag	UNP A0A0U2GPS7
A	363	SER	-	expression tag	UNP A0A0U2GPS7
A	364	LEU	-	expression tag	UNP A0A0U2GPS7
A	365	VAL	-	expression tag	UNP A0A0U2GPS7
A	366	SER	-	expression tag	UNP A0A0U2GPS7
A	367	LEU	-	expression tag	UNP A0A0U2GPS7
A	368	LEU	-	expression tag	UNP A0A0U2GPS7
A	369	SER	-	expression tag	UNP A0A0U2GPS7
A	370	VAL	-	expression tag	UNP A0A0U2GPS7
A	371	LEU	-	expression tag	UNP A0A0U2GPS7
A	372	LEU	-	expression tag	UNP A0A0U2GPS7
A	373	MET	-	expression tag	UNP A0A0U2GPS7
A	374	GLY	-	expression tag	UNP A0A0U2GPS7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	375	CYS	-	expression tag	UNP A0A0U2GPS7
A	376	VAL	-	expression tag	UNP A0A0U2GPS7
A	377	ALA	-	expression tag	UNP A0A0U2GPS7
A	378	GLU	-	expression tag	UNP A0A0U2GPS7
A	379	THR	-	expression tag	UNP A0A0U2GPS7
A	380	GLY	-	expression tag	UNP A0A0U2GPS7
A	381	THR	-	expression tag	UNP A0A0U2GPS7
A	589	GLY	-	expression tag	UNP A0A0U2GPS7
A	590	SER	-	expression tag	UNP A0A0U2GPS7
A	591	LEU	-	expression tag	UNP A0A0U2GPS7
A	592	VAL	-	expression tag	UNP A0A0U2GPS7
A	593	PRO	-	expression tag	UNP A0A0U2GPS7
A	594	ARG	-	expression tag	UNP A0A0U2GPS7
A	595	GLY	-	expression tag	UNP A0A0U2GPS7
A	596	SER	-	expression tag	UNP A0A0U2GPS7
A	597	GLY	-	expression tag	UNP A0A0U2GPS7
A	598	GLY	-	expression tag	UNP A0A0U2GPS7
A	599	SER	-	expression tag	UNP A0A0U2GPS7
A	600	HIS	-	expression tag	UNP A0A0U2GPS7
A	601	HIS	-	expression tag	UNP A0A0U2GPS7
A	602	HIS	-	expression tag	UNP A0A0U2GPS7
A	603	HIS	-	expression tag	UNP A0A0U2GPS7
A	604	HIS	-	expression tag	UNP A0A0U2GPS7
A	605	HIS	-	expression tag	UNP A0A0U2GPS7
A	606	HIS	-	expression tag	UNP A0A0U2GPS7
A	607	HIS	-	expression tag	UNP A0A0U2GPS7
B	350	MET	-	initiating methionine	UNP A0A0U2GPS7
B	351	GLY	-	expression tag	UNP A0A0U2GPS7
B	352	ILE	-	expression tag	UNP A0A0U2GPS7
B	353	LEU	-	expression tag	UNP A0A0U2GPS7
B	354	PRO	-	expression tag	UNP A0A0U2GPS7
B	355	SER	-	expression tag	UNP A0A0U2GPS7
B	356	PRO	-	expression tag	UNP A0A0U2GPS7
B	357	GLY	-	expression tag	UNP A0A0U2GPS7
B	358	MET	-	expression tag	UNP A0A0U2GPS7
B	359	PRO	-	expression tag	UNP A0A0U2GPS7
B	360	ALA	-	expression tag	UNP A0A0U2GPS7
B	361	LEU	-	expression tag	UNP A0A0U2GPS7
B	362	LEU	-	expression tag	UNP A0A0U2GPS7
B	363	SER	-	expression tag	UNP A0A0U2GPS7
B	364	LEU	-	expression tag	UNP A0A0U2GPS7
B	365	VAL	-	expression tag	UNP A0A0U2GPS7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	366	SER	-	expression tag	UNP A0A0U2GPS7
B	367	LEU	-	expression tag	UNP A0A0U2GPS7
B	368	LEU	-	expression tag	UNP A0A0U2GPS7
B	369	SER	-	expression tag	UNP A0A0U2GPS7
B	370	VAL	-	expression tag	UNP A0A0U2GPS7
B	371	LEU	-	expression tag	UNP A0A0U2GPS7
B	372	LEU	-	expression tag	UNP A0A0U2GPS7
B	373	MET	-	expression tag	UNP A0A0U2GPS7
B	374	GLY	-	expression tag	UNP A0A0U2GPS7
B	375	CYS	-	expression tag	UNP A0A0U2GPS7
B	376	VAL	-	expression tag	UNP A0A0U2GPS7
B	377	ALA	-	expression tag	UNP A0A0U2GPS7
B	378	GLU	-	expression tag	UNP A0A0U2GPS7
B	379	THR	-	expression tag	UNP A0A0U2GPS7
B	380	GLY	-	expression tag	UNP A0A0U2GPS7
B	381	THR	-	expression tag	UNP A0A0U2GPS7
B	589	GLY	-	expression tag	UNP A0A0U2GPS7
B	590	SER	-	expression tag	UNP A0A0U2GPS7
B	591	LEU	-	expression tag	UNP A0A0U2GPS7
B	592	VAL	-	expression tag	UNP A0A0U2GPS7
B	593	PRO	-	expression tag	UNP A0A0U2GPS7
B	594	ARG	-	expression tag	UNP A0A0U2GPS7
B	595	GLY	-	expression tag	UNP A0A0U2GPS7
B	596	SER	-	expression tag	UNP A0A0U2GPS7
B	597	GLY	-	expression tag	UNP A0A0U2GPS7
B	598	GLY	-	expression tag	UNP A0A0U2GPS7
B	599	SER	-	expression tag	UNP A0A0U2GPS7
B	600	HIS	-	expression tag	UNP A0A0U2GPS7
B	601	HIS	-	expression tag	UNP A0A0U2GPS7
B	602	HIS	-	expression tag	UNP A0A0U2GPS7
B	603	HIS	-	expression tag	UNP A0A0U2GPS7
B	604	HIS	-	expression tag	UNP A0A0U2GPS7
B	605	HIS	-	expression tag	UNP A0A0U2GPS7
B	606	HIS	-	expression tag	UNP A0A0U2GPS7
B	607	HIS	-	expression tag	UNP A0A0U2GPS7

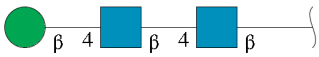
- Molecule 2 is a protein called Designed miniprotein cb_3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	58	Total	C	N	O	0	1	0
			458	288	80	90			
2	D	57	Total	C	N	O	0	0	0
			435	277	75	83			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

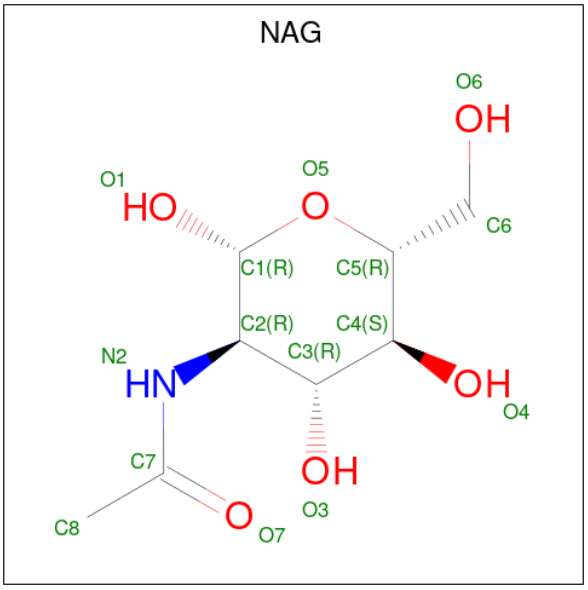
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

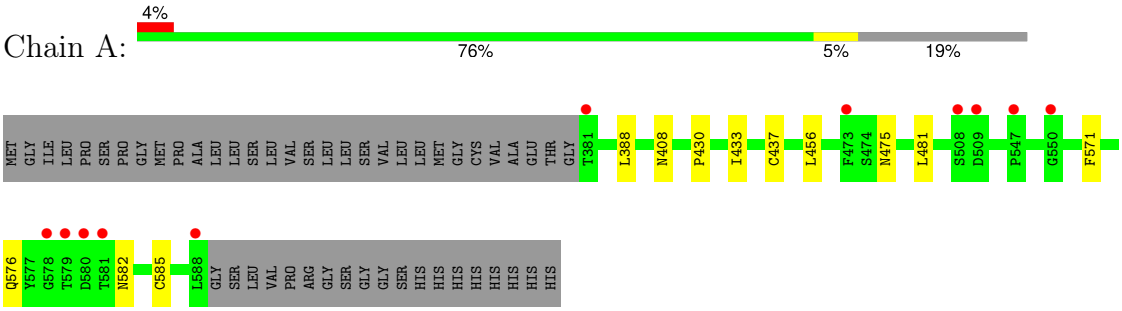
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	115	Total O 115 115	0	0
6	B	154	Total O 154 154	0	0
6	C	24	Total O 24 24	0	0
6	D	13	Total O 13 13	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

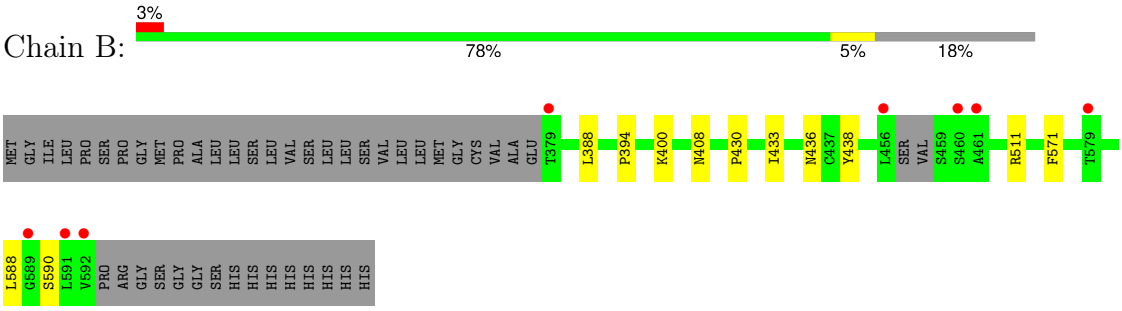
• Molecule 1: Spike glycoprotein

Chain A:



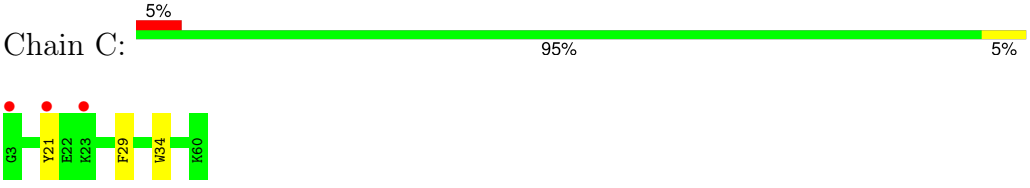
• Molecule 1: Spike glycoprotein

Chain B:



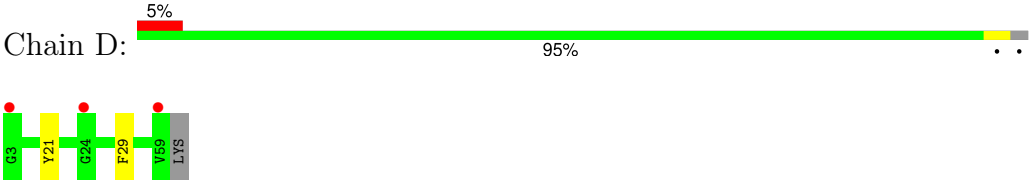
• Molecule 2: Designed miniprotein cb_3

Chain C:



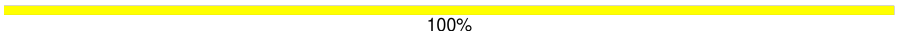
• Molecule 2: Designed miniprotein cb_3

Chain D:



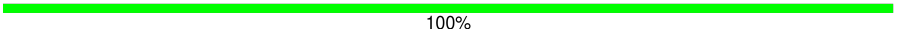
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.62Å 76.29Å 136.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.55 – 1.85 31.55 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.55-1.85) 99.9 (31.55-1.85)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 1.85Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.190 , 0.219 0.190 , 0.217	Depositor DCC
R_{free} test set	2759 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4492	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/1609	0.49	0/2204
1	B	0.32	0/1670	0.52	0/2282
2	C	0.27	0/466	0.37	0/632
2	D	0.22	0/443	0.34	0/601
All	All	0.29	0/4188	0.48	0/5719

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1568	0	1478	6	0
1	B	1630	0	1555	7	0
2	C	458	0	396	2	0
2	D	435	0	381	1	0
3	E	28	0	25	0	0
4	F	39	0	34	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	115	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	154	0	0	1	0
6	C	24	0	0	0	1
6	D	13	0	0	0	1
All	All	4492	0	3895	15	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (15) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HD23	1:A:481:LEU:HD21	1.80	0.64
1:B:388:LEU:HD11	1:B:571:PHE:CE1	2.42	0.54
1:B:394:PRO:HG3	1:B:400:LYS:HG3	1.93	0.50
1:A:437:CYS:HB3	1:A:582:ASN:HB3	1.95	0.48
2:D:21:TYR:HB2	2:D:29:PHE:CD1	2.50	0.47
1:A:388:LEU:HD11	1:A:571:PHE:CE1	2.49	0.47
1:B:436:ASN:HB2	1:B:438:TYR:CZ	2.51	0.46
1:B:430:PRO:O	1:B:433:ILE:HG22	2.17	0.45
1:A:430:PRO:O	1:A:433:ILE:HG22	2.16	0.45
1:A:475:ASN:OD1	1:A:576:GLN:HG2	2.18	0.44
1:B:408[A]:ASN:OD1	6:B:801:HOH:O	2.20	0.44
1:B:511:ARG:HD2	2:C:34:TRP:CE3	2.54	0.42
1:B:588:LEU:HD23	1:B:588:LEU:HA	1.86	0.42
2:C:21:TYR:HB2	2:C:29:PHE:CD1	2.56	0.41
1:A:408:ASN:HA	1:A:585:CYS:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:120:HOH:O	6:D:112:HOH:O[1_565]	2.10	0.10

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	208/258 (81%)	207 (100%)	1 (0%)	0	100	100
1	B	212/258 (82%)	210 (99%)	2 (1%)	0	100	100
2	C	57/58 (98%)	57 (100%)	0	0	100	100
2	D	55/58 (95%)	55 (100%)	0	0	100	100
All	All	532/632 (84%)	529 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	177/230 (77%)	177 (100%)	0	100	100
1	B	188/230 (82%)	187 (100%)	1 (0%)	86	84
2	C	40/50 (80%)	40 (100%)	0	100	100
2	D	37/50 (74%)	37 (100%)	0	100	100
All	All	442/560 (79%)	441 (100%)	1 (0%)	92	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	590	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	ASN
1	B	519	ASN

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Mol	Chain	Res	Type
1	B	566	GLN
1	B	576	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

5 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.71	0	17,19,21	1.00	2 (11%)
3	NAG	E	2	3	14,14,15	0.69	0	17,19,21	1.63	2 (11%)
4	NAG	F	1	1,4	14,14,15	0.39	0	17,19,21	0.42	0
4	NAG	F	2	4	14,14,15	0.38	0	17,19,21	0.45	0
4	BMA	F	3	4	11,11,12	0.27	0	15,15,17	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	NAG	C1-O5-C5	5.16	119.10	112.19
3	E	1	NAG	C1-C2-N2	-2.35	106.74	110.43
3	E	1	NAG	C2-N2-C7	2.20	125.85	122.90
3	E	2	NAG	C4-C3-C2	-2.20	107.80	111.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

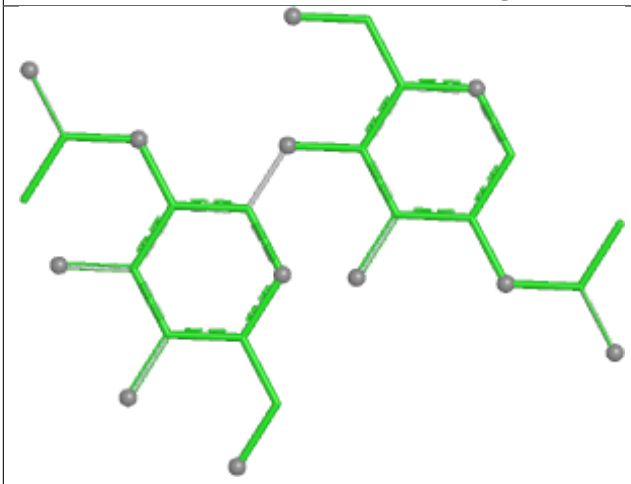
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

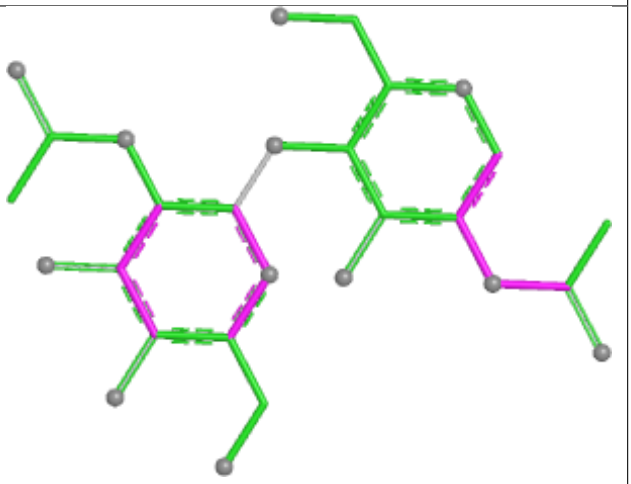
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

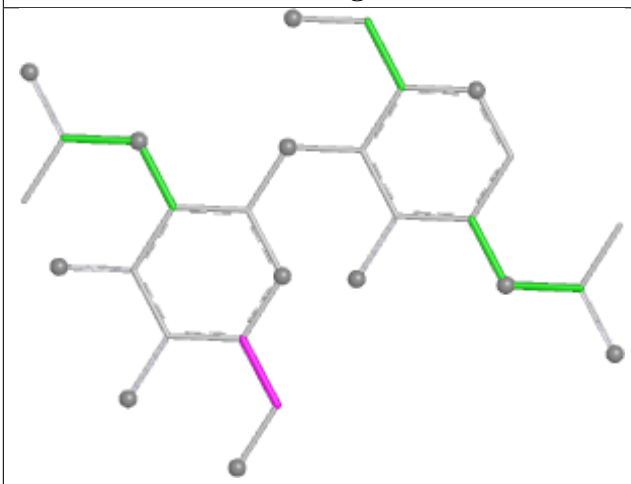
Oligosaccharide Chain E



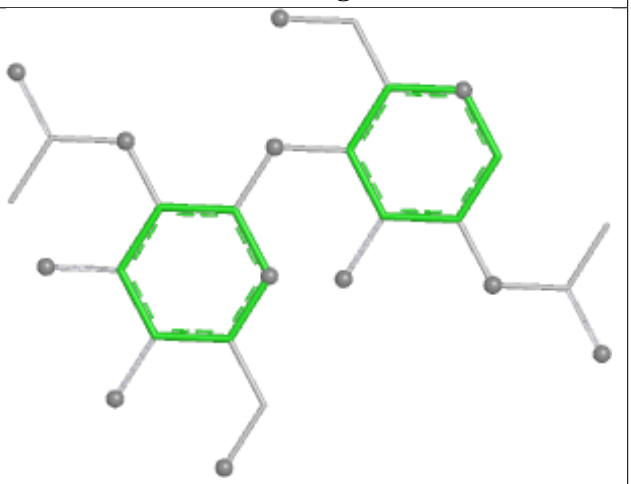
Bond lengths



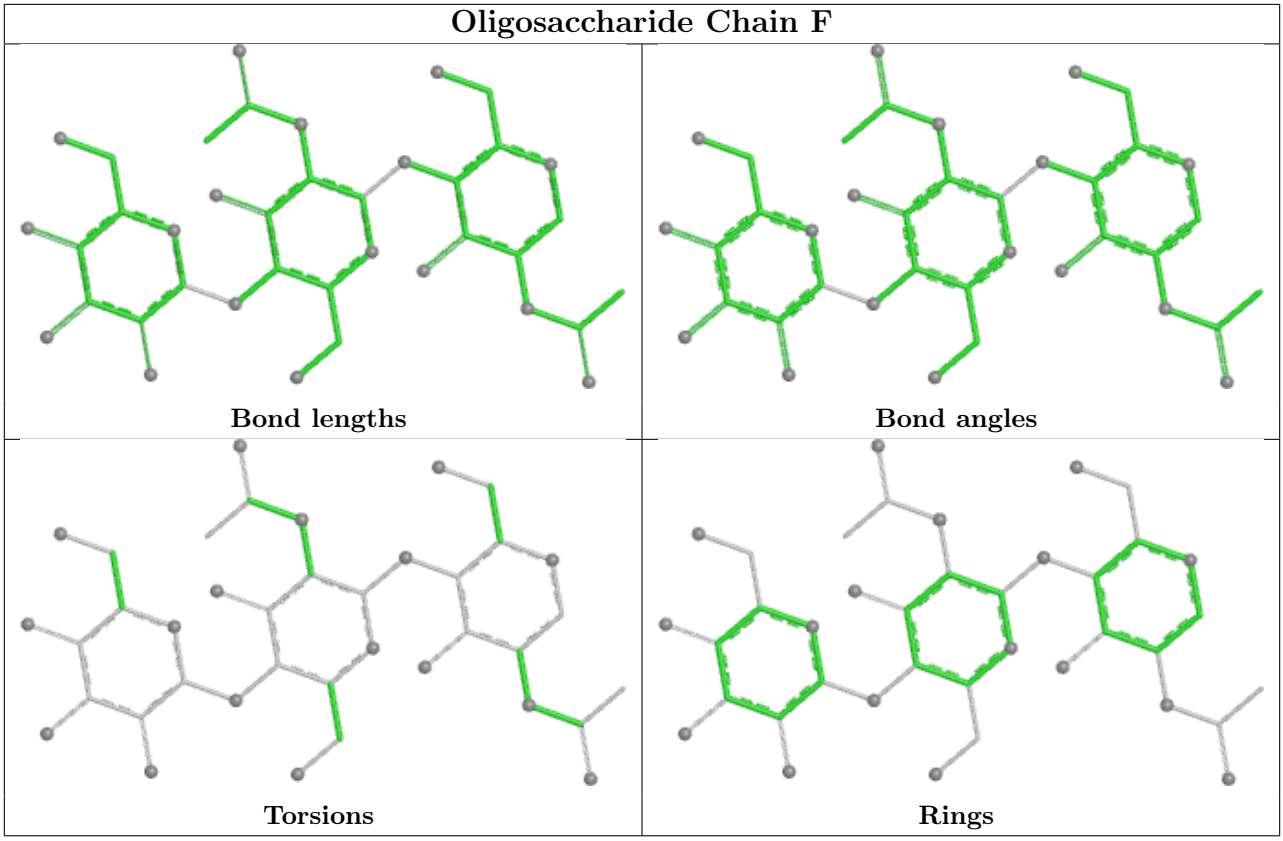
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	701	1	14,14,15	0.71	0	17,19,21	1.11	2 (11%)
5	NAG	A	701	1	14,14,15	0.72	0	17,19,21	0.99	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	701	1	-	0/6/23/26	0/1/1/1
5	NAG	A	701	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	701	NAG	C1-O5-C5	2.56	115.61	112.19
5	B	701	NAG	C2-N2-C7	2.40	126.12	122.90
5	A	701	NAG	C1-O5-C5	2.20	115.13	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

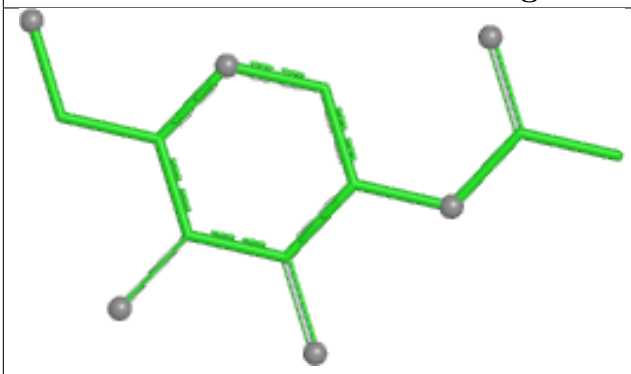
Mol	Chain	Res	Type	Atoms
5	A	701	NAG	C8-C7-N2-C2
5	A	701	NAG	O7-C7-N2-C2

There are no ring outliers.

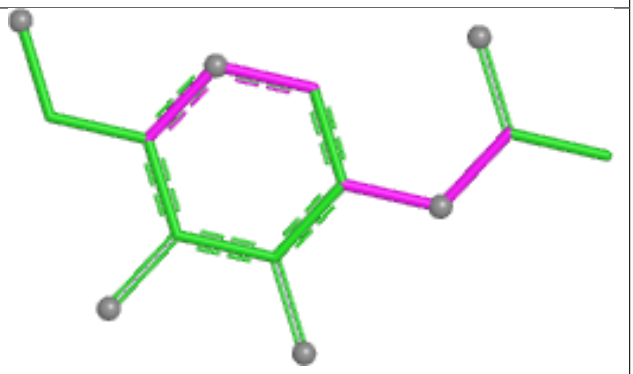
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

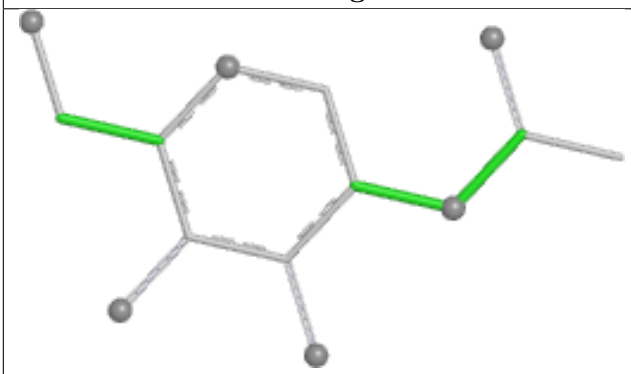
Ligand NAG B 701



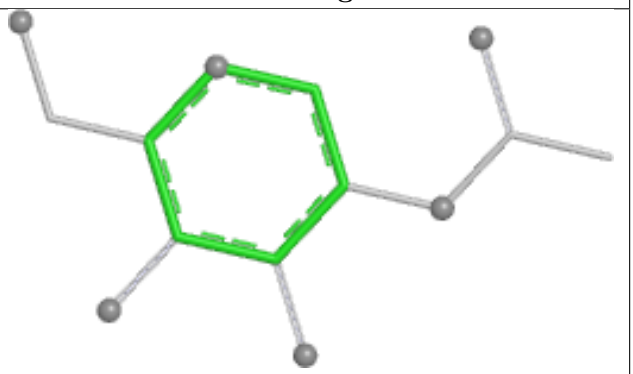
Bond lengths



Bond angles

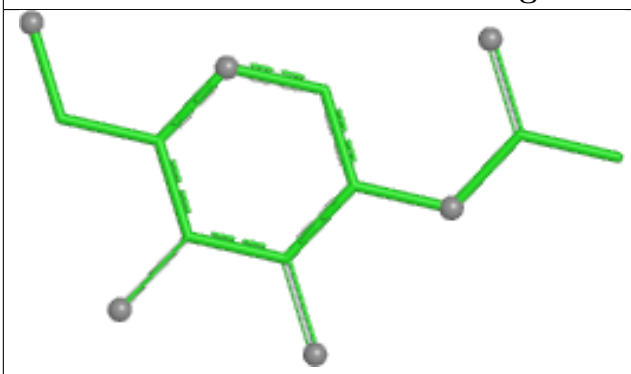


Torsions

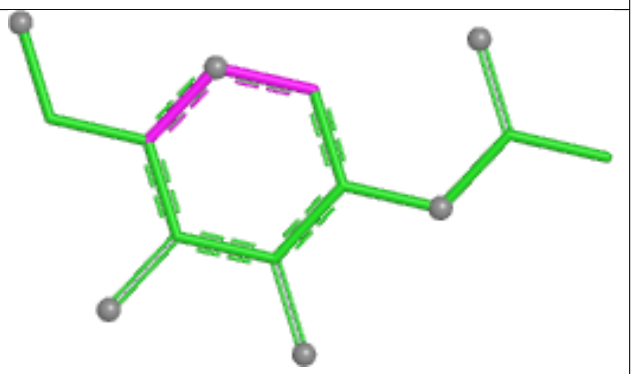


Rings

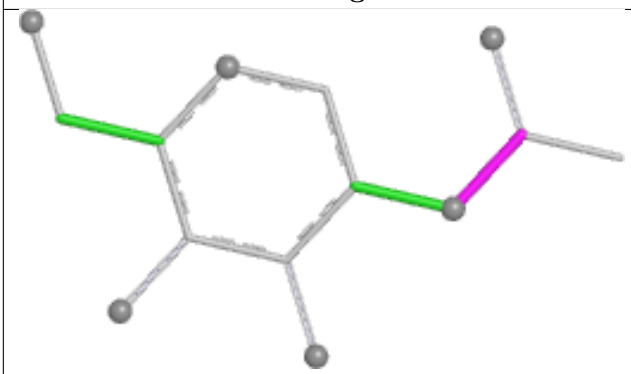
Ligand NAG A 701



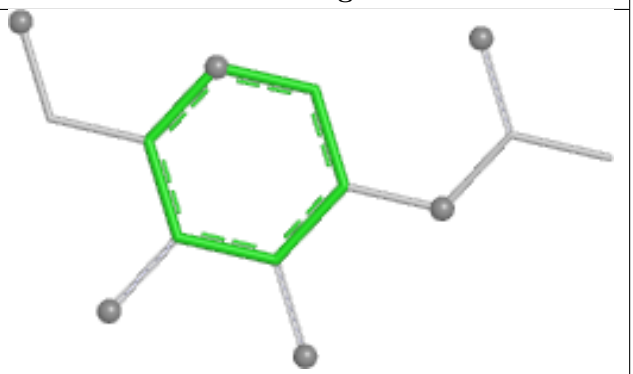
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	208/258 (80%)	0.20	11 (5%)	33	35	16, 36, 63, 89	2 (0%)
1	B	212/258 (82%)	0.05	8 (3%)	44	47	11, 32, 55, 72	4 (1%)
2	C	58/58 (100%)	0.46	3 (5%)	34	35	23, 41, 60, 66	1 (1%)
2	D	57/58 (98%)	0.44	3 (5%)	33	35	31, 44, 64, 68	0
All	All	535/632 (84%)	0.19	25 (4%)	37	39	11, 36, 62, 89	7 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	SER	4.7
1	B	592	VAL	4.7
1	A	581	THR	4.6
1	A	580	ASP	4.1
1	B	591	LEU	4.0
1	B	461	ALA	3.7
2	C	3	GLY	3.6
1	A	578	GLY	3.5
2	D	3	GLY	3.1
1	A	509	ASP	3.1
2	D	59	VAL	2.9
1	A	579	THR	2.6
1	B	579	THR	2.5
1	A	381	THR	2.5
1	A	473	PHE	2.4
2	D	24	GLY	2.3
1	B	589	GLY	2.3
1	A	588	LEU	2.3
2	C	23	LYS	2.2
2	C	21	TYR	2.2
1	B	456	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	379	THR	2.1
1	A	547	PRO	2.1
1	A	508	SER	2.1
1	A	550	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

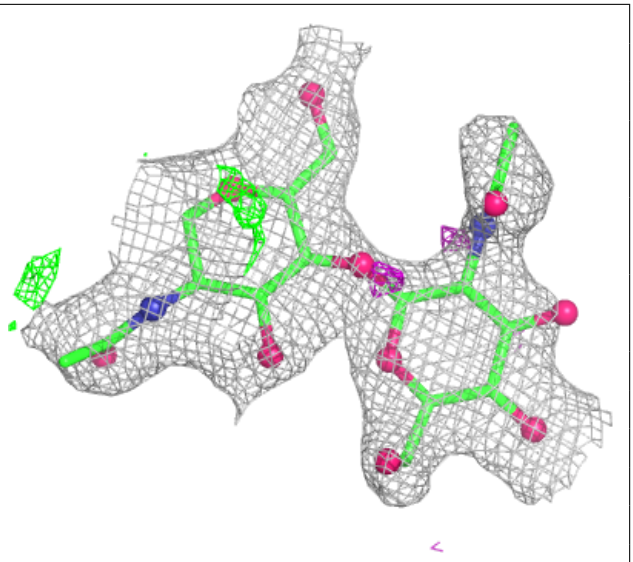
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

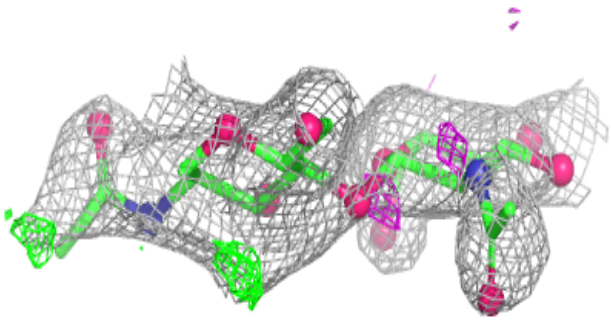
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BMA	F	3	11/12	0.17	0.17	97,99,103,104	0
4	NAG	F	2	14/15	0.69	0.13	58,74,86,93	0
3	NAG	E	1	14/15	0.71	0.14	50,62,69,70	0
3	NAG	E	2	14/15	0.75	0.13	57,63,68,70	0
4	NAG	F	1	14/15	0.82	0.12	42,52,63,63	0

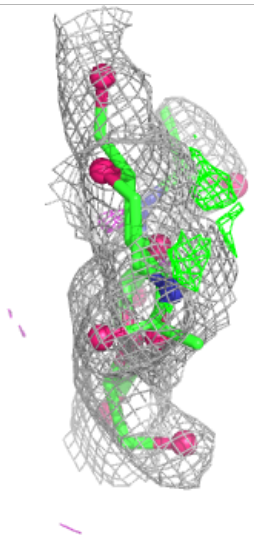
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

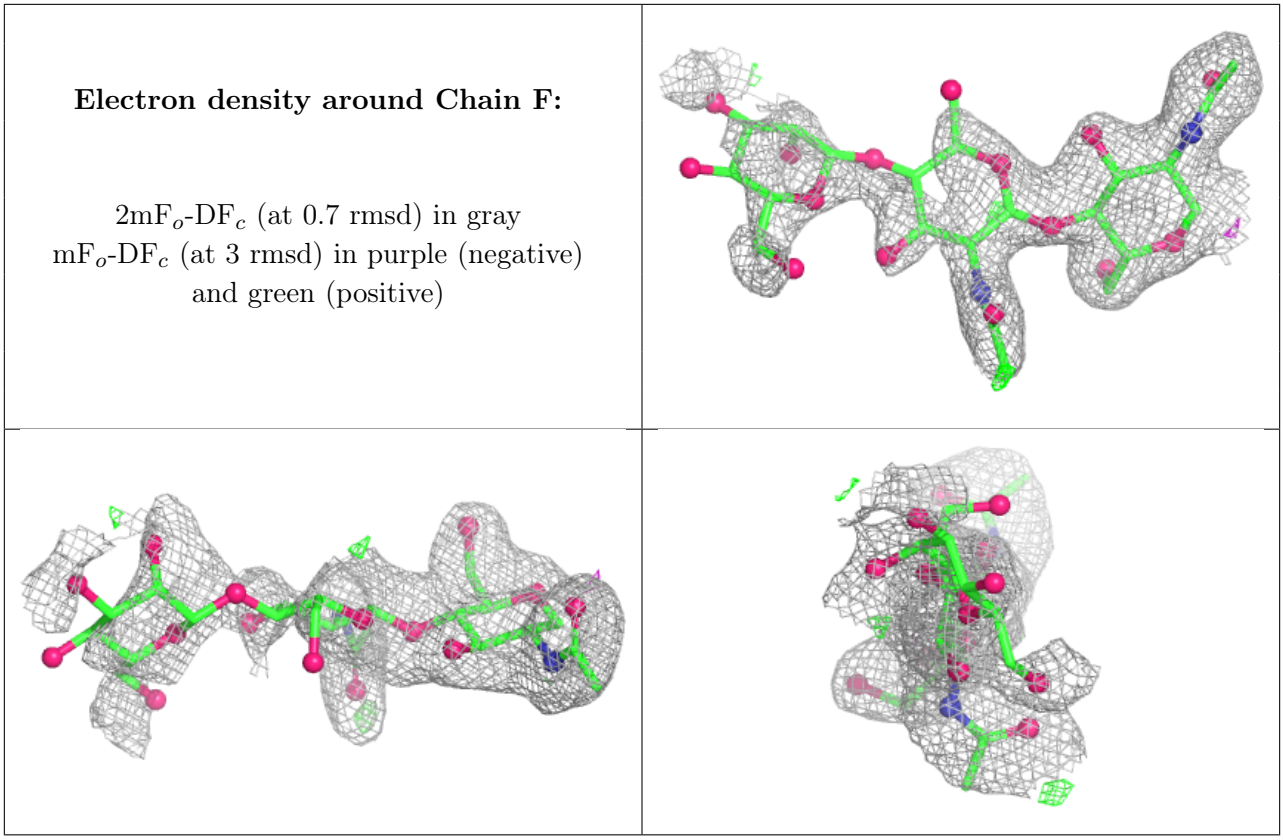






Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

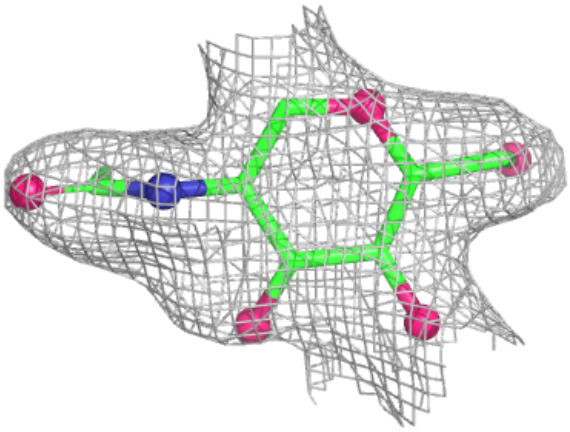
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

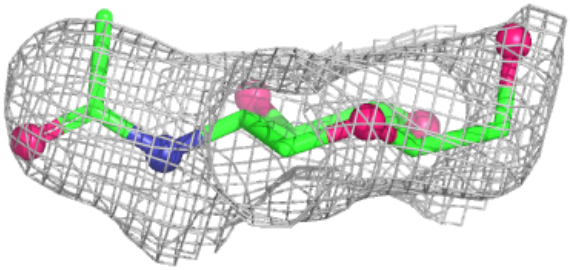
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	A	701	14/15	0.75	0.12	63,70,75,76	0
5	NAG	B	701	14/15	0.79	0.12	56,62,75,77	0

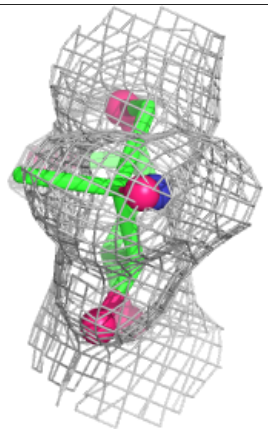
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG A 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

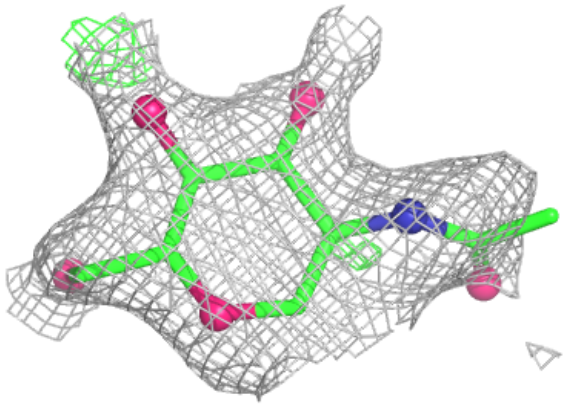


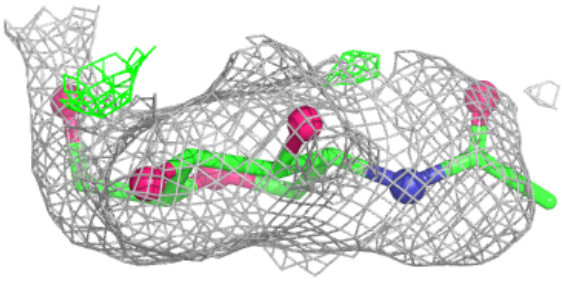


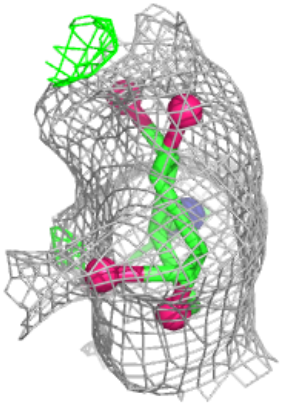


Electron density around NAG B 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.